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Bounds on Scattering Phase Shifts

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LARRY SPRUCH

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Larry Spruch

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Morris Kline
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Project Director

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Abstract

Though the Kato technique for obtaining bounds on the cotangent of the scattering phase shift, $\bar{\eta}_L$, is extremely general and powerful, an integration must be performed which can be quite troublesome, and some preliminary, albeit crude, information about $\bar{\eta}_L$ is required before the method can be applied. It is shown here that in the evaluation of the upper bound on cot $\bar{\eta}_L$, the integration can often be eliminated without any significant increase in the value of the upper bound. It is also shown that the Kato formalism is often useful even when one does not possess the necessary a priori knowledge of $\bar{\eta}_L$; under realistic specified conditions, a bound can be obtained on $\bar{\eta}_L$ even when a bound cannot be obtained on cot $\bar{\eta}_L$. Further, a 'bootstrap technique' is introduced whereby this bound on $\bar{\eta}_L$ can be improved. The bound on $\bar{\eta}_L$ is of interest in its own right. It may also help to provide the preliminary information necessary for the determination of bounds on cot $\bar{\eta}_L$.

It is shown that if the potential $V(r)$ is non-positive, $\bar{\eta}_{L+}$ and/or $|\bar{\eta}_{L-}|$ must be larger than the Born phase shift η_{L+B}, where $\bar{\eta}_{L\pm}$ are the phase shifts associated with $\mp V$; if $V(r) \leq 0$ and if $|\bar{\eta}_{L\pm}| < \pi$, then $\cot \bar{\eta}_{L+} - \cot \bar{\eta}_{L-} \leq 2 \cot \eta_{L+B}$. A slight generalization of the Schwinger integral variational principle gives similar results for phases related to $V \pm U$.

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1. Introduction

Variational techniques have proved invaluable in scattering theory, in the evaluation of phase shifts, for example. They nevertheless suffer from the serious disadvantage, compared to the corresponding variational calculations of binding energies, for instance, that they do not provide a bound on the phase shift. This disadvantage is most pronounced in problems of such difficulty that one cannot guess at a reasonable form for the trial function, though it is precisely for those problems that variational techniques are potentially most valuable. (We might for example be interested in a particular problem of scattering by a compound system which could not readily be handled by a machine). For a poor trial function, the second order error involved in the variational calculation is not necessarily small. Further, there is the disheartening feature that the inclusion of additional parameters into the trial function may give worse rather than better results.

For these reasons, the general and powerful (and elegant) technique introduced by Kato[1] for obtaining upper and lower bounds on cot $(\bar{\eta}_L - \theta)$ is of considerable significance. For non-relativistic scattering by a central field, Kato deduced the inequality

$$(1.1)\qquad -\alpha_{\theta L}^{-1}\,\varepsilon_{\theta L}^{2} \le k\cot(\bar{\eta}_L - \theta) - k\cot(\eta_L - \theta) + \int u_{\theta L}\mathcal{L}_L\, u_{\theta L}\, dr \le \beta_{\theta L}^{-1}\,\varepsilon_{\theta L}^{2},$$

where

$$(1.2)\qquad \varepsilon_{\theta L}^{2} = \int \rho^{-1}\,(\mathcal{L}_L\, u_{\theta L})^{2}\, dr.$$

The generality of the method consists in the fact that there are no restrictions on the central potential; in principle, it can also be applied to more complicated problems such as the scattering by a compound system. The power of the method lies in the latitude that one has in the choice of the normalization, θ, the trial function, $u_{\theta L}$, and the weight factor, ρ.

There remain nevertheless two disturbing questions. The first is the practical question concerning the difficulty of performing the integration that appears in equation (1.2). The second question, a more serious one in principle, is whether one can in fact determine the eigenvalues $\alpha_{\theta L}$ and $\beta_{\theta L}$, or bounds on them which preserve the inequality. Now, it is known[1],[2] that there is a wide variety of central potentials for which neither of the two questions prove to be very serious. In these cases, the integrals are not really too tedious, and it is not very difficult to obtain bounds on $\alpha_{\theta L}$ and $\beta_{\theta L}$. On the other hand, in scattering by a compound system, for example, these questions assume much more serious proportions. As is not too surprising, other such questions arise in an attempt to obtain bounds on the phase shift for scattering by a compound system. These will be treated at a later date. It is more profitable to examine scattering by a fixed potential first, but from a point of view such that the results will prove useful for application to scattering by a compound system. Thus, techniques are sought whereby it will not be necessary to evaluate the integral in (1.2), since for scattering by a compound system the integration of the analogue of (1.2) may well be prohibitively laborious. Further, we seek techniques by means of which one can obtain $\alpha_{\theta L}$ and/or $\beta_{\theta L}$ with a minimum of a priori information about $\bar{\eta}_L$, or, assuming that one cannot obtain $\alpha_{\theta L}$ or $\beta_{\theta L}$, we seek any information which can still be extracted from the Kato formalism. (In the case of a fixed central potential, bounds on $\alpha_{\theta L}$ and $\beta_{\theta L}$ can generally be determined by comparison of the given potential with known solvable potentials[1],[2]; this is not generally possible in the case of scattering by a compound system, since there are no such realistic solvable potentials).

With regard to the first question, concerning the elimination of the integration, we note that under specified conditions[1],[2] $\beta_{\theta L}$ is infinite. Under these circumstances, for the purposes of obtaining an upper bound on $\cot(\bar{\eta}_L - \theta)$, the integration need not be performed. The conditions include the requirement that the potential be of a solvable form beyond some point a. We consider for the moment the simplest such example, that of a potential which vanishes identically beyond the point a. This suggests[2], for a 'potential' $W(r)$ which is non-negative but which does not vanish identically, that one define a cut-off potential $W^c(r) = W(r) \Sigma(a-r)$, where $\Sigma(a-r)$ is a step function. By the appropriate choice of a, one can cause the $\beta^c_{\theta L}$, associated with $W^c(r)$, to be infinite, in which case $\bar{\eta}^c_L$, the L-th phase shift associated with $W^c(r)$, can be bounded from above without performing the complicated integration. Since $W(r) \geq W^c(r)$, it follows that $\bar{\eta}_L > \bar{\eta}^c_L$, so that the bound obtained on $\bar{\eta}^c_L$ serves as a bound on $\bar{\eta}_L$ as well. While this has been shown to be a reasonable procedure[2] in general, there is sometimes a considerable loss in accuracy, in that it may be necessary to choose a rather small value of a. The difference between W and W^c may then be considerable, in which case even a close bound on $\bar{\eta}_L^c$ will be a poor bound on $\bar{\eta}_L$. It will be shown in Section 3 that the introduction of a constraint on the trial function, $u_{\theta L}$, makes possible an increase in the value of a, thereby decreasing the difference between W and W^c and therefore between $\bar{\eta}_L$ and $\bar{\eta}_L^c$, and making it possible to obtain a better upper bound on $\bar{\eta}_L$. Since it turns out that the constraint on $u_{\theta L}$ is almost always satisfied automatically, there is no real loss of freedom in the choice of $u_{\theta L}$.

Since there does not seem to be any way of eliminating the troublesome integral when one seeks a lower bound on $\cot(\bar{\eta}_L - \theta)$, it is only the upper bound which can ever be obtained relatively simply. This upper bound is of course of interest in its own right; there is in addition the pleasant feature associated with the presence of even only one bound that the inclusion of more free parameters in the trial function guarantees an improved result.

It will also be shown in Section 3 that it is still very profitable to introduce the constraint on $u_{\theta L}$ where one must evaluate the integral, or where one prefers to evaluate the integral rather than lose any accuracy at all by introducing $W^c(r)$. If, as is usually the case, the constraint is automatically satisfied, one obtains an improved bound, as compared to that given in the formulation of Kato, without doing any additional calculation.

Turning now to the second question, concerning the prior knowledge of $\bar{\eta}_L$, we assume, in line with the previous discussion, that so little is known about $\bar{\eta}_L$ that $\alpha_{\theta L}$ and $\beta_{\theta L}$ cannot be determined. Even though one cannot then obtain a bound on $\cot(\bar{\eta}_L - \theta)$, it will be shown in Section 4 that under realistic specified conditions, the Kato method does give a bound on $\bar{\eta}_L$ itself. Further, a 'bootstrap technique' will be introduced in Section 5 whereby this bound on $\bar{\eta}_L$ may successively be improved. The bound on $\bar{\eta}_L$ is of course of interest in its own right; it may also help to provide the preliminary information necessary for the application of the Kato method to the determination of bounds on $\cot(\bar{\eta}_L - \theta)$.

In Section 2, a property of the Schwinger integral variational principle deduced by Kato will be used to develop a very simple but useful inequality involving the phases $\bar{\eta}_{L\pm}$ associated with $\pm W(r)$, and the Born phase shift. A similar inequality is deduced involving phases related to $W(r) \pm U(r)$ by starting with a slight generalization of the Schwinger principle.

2. Equal and opposite potentials

A. Phase shifts associated with ± W. Assume that the L-th phase shift $\bar{\eta}_{L+}$ associated with $W(r) \geq 0$ satisfies $\bar{\eta}_{L+} < \pi$. Under these circumstances, as was shown by Kato, a bound on k cot $\bar{\eta}_{L+}$ is provided by the Schwinger integral variational principle, that is,

$$(2.1) \qquad k \cot \bar{\eta}_{L+} \leq \int Wv^2_{L+}\, dr - \int dr \int dr'\, v_{L+}\, WG_L\, Wv_{L+},$$

where the only restriction on the trial function $v_{L+}(r)$ is that it must satisfy

$$(2.2) \qquad k^{-1} \int krj_L(kr)W(r)v_{L+}(r)dr = 1,$$

and where the free particle Green's function $G_L(r,r')$ is given by

$$(2.3) \qquad G_L(r,r') = -k^{-1}krj_L(kr)\ kr,n_L(kr).$$

Assume further that the L-th phase shift $\bar{\eta}_{L-}$ associated with $-W(r)$ satisfies $\bar{\eta}_{L-} > -\pi$. Then, similarly

$$(2.4) \qquad k \cot \bar{\eta}_{L-} \geq \int (-W)v^2_{L-}dr - \int dr \int dr'\, v_{L-}(-W)G_L(-W)v_{L-},$$

where the only restriction on $v_{L-}(r)$ is that it must satisfy

$$(2.5) \qquad k^{-1} \int krj_L(kr)\left[-W(r)\right]\, v_{L-}(r)dr = 1.$$

From equations (2.2) and (2.5), it is clear that it is permissible to choose $v_{L-}(r) = -v_{L+}(r)$. If this is done, it follows from (2.1) and (2.4) that

$$(2.6) \qquad \cot \bar{\eta}_{L+} - \cot \bar{\eta}_{L-} \leq 2k^{-1} \int W(r)\, v^2_{L+}(r)dr,$$

where $v_{L+}(r)$ satisfies (2.2). Equation (2.6), which gives a bound for one of the two phases if the other is known, has the pleasant feature that it does not contain $G_L(r,r')$; the question as to whether it is likely to provide a useful bound remains to be discussed.

The choice of $v_{L+}(r)$ will now be considered. We can write

$$(2.7) \qquad \cot \bar{\eta}_{L+} - \cot \bar{\eta}_{L-} \leq F\left[v_{L+}\right],$$

where the functional $F[v_{L+}]$ is given by

$$(2.8) \qquad F\left[v_{L+}\right] = 2k \int Wv^2_{L+}dr\left[\int krj_L(kr)Wv_{L+}dr\right]^{-2},$$

and where there are now no restrictions whatever on $v_{L+}(r)$. If, in the denominator, we use the fact that $W(r) \geq 0$ to write $W(r) = W^{1/2}(r)W^{1/2}(r)$, an application of Schwarz' theorem gives

$$\left[\int krj_L(kr)Wv_{L+}dr\right]^2 \leq \int\left[krj_L(kr)\right]^2 Wdr \int Wv^2_{L+}\, dr.$$

It then follows that

$$(2.9) \qquad F\left[v_{L+}\right] \geq 2k \left\langle \int\left[krj_L(kr)\right]^2 Wdr \right\rangle^{-1} = 2 \cot \eta_{L+B} = -2 \cot \eta_{L-B},$$

where $\eta_{L\pm B}$ is the L-th phase shift for $\pm W$ in the Born approximation. On the other hand,

$$(2.10) \qquad F\left[v_{L+} = krj_L(kr)\right] = 2 \cot \eta_{L+B}.$$

It follows from equations (2.7), (2.9), and (2.10) that once one has chosen $v_{L-}(r) = -v_{L+}(r)$, the best possible choice for $v_{L+}(r)$ is $krj_L(kr)$. In summary, we see that if $W(r) \geq 0$, if $\bar{\eta}_{L+} < \pi$, and if $\bar{\eta}_{L-} > -\pi$, then

$$(2.11) \qquad \cot \bar{\eta}_{L+} - \cot \bar{\eta}_{L-} \leq 2 \cot \eta_{L+B}.$$

One might expect the bound given by (2.11) to be exceedingly poor, because of the choice $v_{L-}(r) = -v_{L+}(r)$. Actually, due to the presence of the Green's function in the Schwinger variational principle, it is somewhat misleading to think of $v_{L+}(r)$ and $v_{L-}(r)$ as the trial functions. Thus, the trial functions in the Kato formalism which give rise to the Schwinger variational principle are

$$(2.12) \qquad u_{oL\pm}(r) = \cot \eta_{L\pm} krj_L(kr) + \int G_L(\pm W)\, v_{L\pm}dr'.$$

Then, with $v_{L+}(r) = krj_L(kr) = -v_{L-}(r)$, we have

$$(2.13) \qquad u_{oL\pm}(r) = \cot\eta_{L\pm}\, krj_L(kr) + \int G_L(r,r')W(r')kr'j_L(kr')dr'.$$

The choices of η_{L+} and η_{L-} are each completely arbitrary, so that there can be considerable difference between u_{oL+} and u_{oL-}. More important is the fact that if $\bar{\eta}_{L+}$ and $|\bar{\eta}_{L-}|$ are not too large, u_{oL+} and u_{oL-} should be fairly reasonable trial functions. (It is to be noted that if η_{L+} and $|\eta_{L-}|$ are less than $\frac{1}{2}\pi$, $\cot\eta_{L+}$ and $\cot\eta_{L-}$ will be of opposite sign, so that the 'correction terms' involving the integral appear in (2.13) for u_{oL+} and u_{oL-} in effect with opposite signs, as they should). Equation (2.11) should not therefore give too crude a bound for $\bar{\eta}_{L+}$ and $|\bar{\eta}_{L-}|$ not too large. As examples, we have plotted in Figure 1 the bounds on, and the exact values of, $\cot\bar{\eta}_{L+} - \cot\bar{\eta}_{L-}$ for the case of a square well for a few sets of values of the parameters. It can be seen that, qualitatively, the bound becomes crude only when $\bar{\eta}_{L+}$ or $|\bar{\eta}_{L-}|$ is of the order of $\frac{1}{2}\pi$.

When equation (2.11) is valid, $\bar{\eta}_{L+}$ of $|\bar{\eta}_{L-}|$, or both, must be larger than η_{L+B}. Since η_{L+B} as defined by (2.9) is less than π, (in fact it is less than $\frac{\pi}{2}$), it follows without any prior information about $\bar{\eta}_{L+}$ or $|\bar{\eta}_{L-}|$, that if $W(r) \geq 0$, then at least one of $\bar{\eta}_{L+}$ and $|\bar{\eta}_{L-}|$ must be larger than η_{L+B}.

B. Phase shifts associated with W ± U. The above results can be generalized somewhat. Let $W(r)$ be a solvable 'potential'; in particular, let the phase shift $\bar{\eta}_L$, the 'absolute normalization' solution $\bar{f}_L(r)$, and the (irregular) solution $\bar{g}_L(r)$ which has the asymptotic form

$$(2.14) \qquad \bar{g}_L(r) \rightarrow -\cos(kr - \tfrac{1}{2}L\pi + \bar{\eta}_L)$$

be known. Let the L-th phase shifts associated with W ± U be $\bar{\eta}_L \pm \Delta\bar{\eta}_{L\pm}$, respectively. (The $\Delta\bar{\eta}_{L\pm}$ are of course not the phase shifts associated with ± U). No assumptions are made regarding the relative magnitudes or ranges of W and U. We seek a simple inequality of the form of equation (2.11) which involves the $\Delta\bar{\eta}_{L\pm}$.

Kato determined bounds not only for phase shifts but for 'additional phase shifts' of the type $\Delta\bar{\eta}_{L\pm}$. If $U(r) \geq 0$, (no such assumption must be made for $W(r)$), and if $\Delta\bar{\eta}_{L+} < \pi$, the choice $\rho = U$ and $\theta = 0$ gives $\beta_{OL+} = 1$, and the

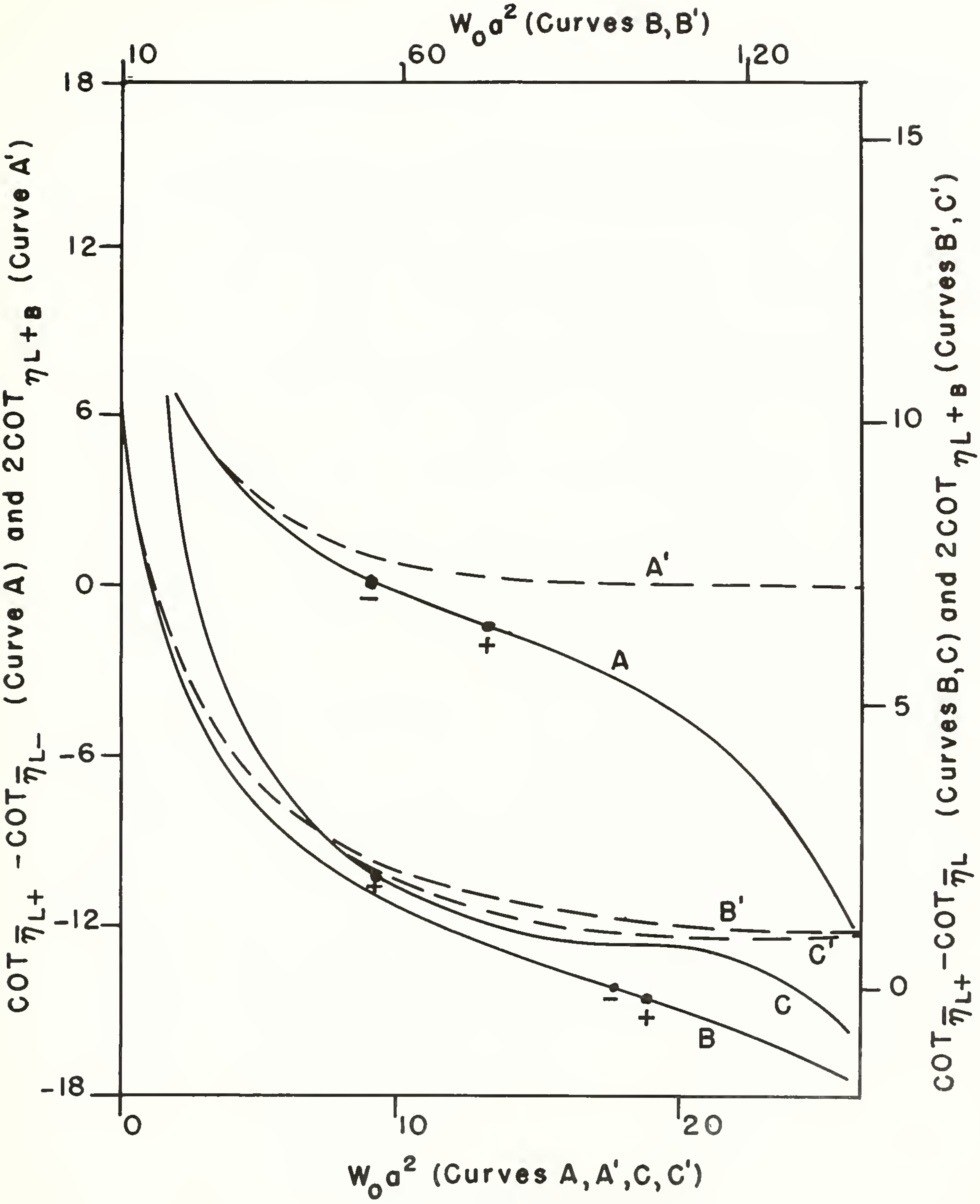

Figure I

A comparison of $\cot\bar{\eta}_{L+} - \cot\bar{\eta}_{L-}$ (the solid curves) with its upper bound, $2\cot\eta_{L+B}$ (the dashed curves), for the case of a square well of strength W_0 and range a. $\bar{\eta}_{L\pm}$ and η_{L+B} are the exact phase shifts associated with ±W and the Born approximation phase shift, respectively. The values of L and of ka for curves A, B, and C are L = 0, 0, and 1, and ka = $5\pi/4$, 10π, and 2, respectively. The plus and minus signs on the graph represent the points at which $\bar{\eta}_{L+} = \frac{1}{2}\pi$ and at which $\bar{\eta}_{L-} = -\frac{1}{2}\pi$.

bound becomes

$$(2.15) \qquad k \cot \Delta \bar{\eta}_{L+} \leq k \cot \Delta \eta_{L+} - \int u_{0L+} \mathcal{L}_{L+} u_{0L+} dr + \int U^{-1} (\mathcal{L}_{L+} u_{0L+} dr)^2$$

where

$$\mathcal{L}_{L\pm} = \frac{d^2}{dr^2} + k^2 - \frac{L(L+1)}{r^2} + W \pm U,$$

and where the trial function u_{0L+} must vanish at the origin and must have the asymptotic form

$$(2.16) \qquad u_{0L+} \rightarrow \cos(kr - \tfrac{1}{2} L \pi + \bar{\eta}_L) + \cot \Delta \eta_{L+} \sin(kr - \tfrac{1}{2} L\pi + \bar{\eta}_L).$$

Choose

$$(2.17) \qquad u_{0L+}(r) = \cot \Delta \eta_{L+} \bar{f}_L(r) + \int \mathcal{G}_L(r,r') U(r') v_{L+}(r') dr',$$

where the Green's function $\mathcal{G}_L$ is given by

$$(2.18) \qquad \mathcal{G}_L(r,r') = -k^{-1} \bar{f}_L(r_<) \, \bar{g}_L(r_>),$$

and where the only restriction on v_{L+} is the normalization condition

$$(2.19) \qquad k^{-1} \int \bar{f}_L(r) \, U(r) \, v_{L+}(r) dr = 1.$$

Equation (2.15) then becomes

$$(2.20) \qquad \cot \Delta \bar{\eta}_{L+} \leq k(\int U v^2_{L+} dr - \int v_{L+} U \mathcal{G}_L U v_{L+} dr)(\int U \bar{f}_L v_{L+} dr)^{-2}.$$

The right side of (2.20) is a slight generalization of the Schwinger integral variational expression for the phase shift. It does not seem to have appeared in print, though the corresponding generalization of the Schwinger integral variational principle for the scattering amplitude has been given (cf. for example [3]).

Equation (2.20) will not in fact often be useful as it stands, due to the presence of the Green's function. It can be of use, however, when employed in conjunction with the corresponding bound on cot $\Delta \bar{\eta}_{L-}$ which arises if $\Delta \bar{\eta}_{L-} > -\pi$. The latter bound involves the trial function v_{L-} which must satisfy the normalization condition

(2.21) $$k^{-1} \int \bar{f}_L(-U)v_{L-}dr = 1.$$

With the choice $v_{L-} = -v_{L+}$, which is consistent with equations (2.19) and (2.21), equation (2.20) and its analogue give

$$\cot \Delta \bar{\eta}_{L+} - \cot \Delta \bar{\eta}_{L-} \leq 2k \left(\int Uv^2_{L+}dr\right)\left(\int U\bar{f}_L v_{L+}dr\right)^{-2}.$$

An analysis identical to that of subsection A shows that once one has chosen $v_{L-} = -v_{1+}$, the best possible choice of v_{L+} is

$$v_{L+}(r) = \bar{f}_L(r),$$

so that finally

(2.22) $$\cot \Delta \bar{\eta}_{L+} - \cot \Delta \bar{\eta}_{L-} \leq 2k\left(\int U\bar{f}^2_L \, dr\right)^{-1}.$$

Equation (2.22) is clearly a generalization of (2.11), reducing to it for $W \pm U \to \pm W$, that is, for $W \to 0$ and $U \to W$). Note that if (2.22) is to be used but (2.20) is not, it is not necessary to find $\bar{g}_L(r)$.

Equation (2.22) can be expected to give a useful bound, if, roughly speaking, $\Delta \bar{\eta}_{L+}$ and $|\Delta \bar{\eta}_{L-}|$ are each rather less than $\frac{1}{2}\pi$. The argument is the same as that which follows (2.11).

Equations (2.11) and (2.22) have the virtue that the bounds are simple to calculate, for they do not involve the Green's function, and yet the bounds differ from the true value by a second-order term, since they arise from variational forms.

3. Introduction of $_2\beta_{\theta L}$

A. Advantage of introducing $_2\beta_{\theta L}$. By definition, $-\beta_{\theta L}$ is that negative eigenvalue $\mu_{m'L}$ which is smallest in absolute magnitude, so that

(3.1) $$(-\mu_{mL})^{-1} \leq (\beta_{\theta L})^{-1}, \text{ for all } m.$$

(The value of m' depends upon the problem under consideration.) The second-order error term in the Kato variational principle is given by*

---

*A factor of k is missing from some of Kato's formulae, but not from any of his final results.

$$(3.2) \qquad \int w_{\theta L} \mathcal{L}_L w_{\theta L} dr = k \sum_m (-\mu_{mL})^{-1} b^2_{mL},$$

where w is the difference between the trial function and the exact function, where

$$(3.3) \qquad \sum_m b^2_{mL} = k^{-1} \int \rho^{-1} (\mathcal{L}_L u_{\theta L})^2 dr = k^{-1} \varepsilon^2_{\theta L},$$

and where

$$(3.4) \qquad b_{mL} = k^{-1} \int \phi_{mL} \mathcal{L}_L u_{\theta L} dr$$

$$(3.5) \qquad = -\mu_{mL} k^{-1} \int w_{\theta L} \rho \phi_{mL} dr.$$

The ϕ_{mL} are the eigenfunctions of the associated eigenvalue problem. It follows that

$$(3.6) \qquad \int w_{\theta L} \mathcal{L}_L w_{\theta L} dr \leq (\beta_{\theta L})^{-1} \int \rho^{-1} (\mathcal{L}_L u_{\theta L})^2 \, dr.$$

It will be shown later that it is often possible to choose the trial function $u_{\theta L}$ in such a way that $b_{m'L} = 0$. (This is certainly not always possible, for one cannot generally solve for $\phi_{m'L}$). In those cases for which $b_{m'L} = 0$, equation (3.2) becomes

$$(3.7) \qquad \int w_{\theta L} \mathcal{L}_L w_{\theta L} dr = k \sum{}' (-\mu_{mL})^{-1} b^2_{mL},$$

where the prime on the sum denotes the exclusion of the value m = m', while equation (3.3) becomes

$$(3.8) \qquad \sum{}' b^2_{mL} = k^{-1} \int \rho^{-1} (\mathcal{L}_L u_{\theta L})^2 dr.$$

We now define

$$(3.9) \qquad {}_2\beta_{\theta L} = -\mu_{m'-1,L} \quad ,$$

so that $-{}_2\beta_{\theta L}$ is the negative eigenvalue which is second smallest in absolute magnitude, whence

$$(3.10) \qquad (-\mu_{mL})^{-1} \leq ({}_2\beta_{OL})^{-1}, \quad m \neq m',$$

and it follows, if $b_{m'L} = 0$, that

$$(3.11) \qquad \int w_{\theta L} \mathcal{L}_L w_{\theta L} dr \leq ({}_2\beta_{\theta L})^{-1} \int \rho^{-1} (\mathcal{L}_L u_{\theta L})^2 dr.$$

There are three quite different possible advantages associated with (3.11) as opposed to (3.6).

(a) There is the simple fact that ${}_2\beta_{\theta L}$ is larger than $\beta_{\theta L}$.

(b) In the replacement of $W(r)$ by a cut-off 'potential', $W^c(r)$, which enables one to drop the difficult second-order error integral, it will be possible to choose a larger value of the cut-off point a.

(c) There are circumstances for which ${}_2\beta_{\theta L}$ is infinite while $\beta_{\theta L}$ is finite.

Examples of these three cases will be treated in sub-sections C, D, and E, respectively. Firstly, however, we will demonstrate with an example that there are in fact cases for which one can arrange to have $b_{m'L} = 0$.

B. Possibility of introducing ${}_2\beta_{\theta L}$. There exists one particularly important case for which it is trivial to solve for $\phi_{m'L}$, namely, that of a non-negative $W(r)$ whose L-th phase shift is less than π. For the choice $\rho = W$ and $\theta = 0$, a solution of the associated eigenvalue problem which satisfies the necessary boundary and normalization conditions is

$$(3.12) \qquad \phi_{m'L} = \phi_{0L} = N\, kr j_L(kr),$$

where the dimensionless constant N is determined from the relation

$$(3.13) \qquad k^{-1} \int \left[N\, kr j_L(kr)\right]^2 W(r) dr = 1.$$

(In this case, $\beta_{m'L} = \beta_{0L} = -\mu_{0L} = 1$, and ${}_2\beta_{0L} = -\mu_{-1,L}$ is greater than one).

It follows from equation (3.5) that

$$(3.14) \qquad b_{m'L} = b_{0L} = k^{-1} N \int (u_{0L} - \bar{u}_{0L})\, W\, kr j_L(kr) dr.$$

It is then a consequence of the relation

$$(3.15) \qquad \int \bar{u}_{0L} W\, kr j_L(kr) dr = k,$$

which is just the usual exact expression for k sin $\bar{\eta}_L$, written with $\theta = 0$ normalization rather than absolute normalization, that $b_{m'L} = b_{0L} = 0$ if u_{0L} satisfies

$$(3.16) \qquad \int u_{0L} W\, krj_L(kr)dr = k$$

as well as the usual boundary conditions. Equation (3.16) is to be satisfied by adjustment of the parameters contained in u_{0L}. (Alternatively, it is possible to choose a trial function v_{0L} which satisfies the necessary boundary conditions, and then to subtract from v_{0L} that component which is not orthogonal with weight factor $\rho = W$ to ϕ_{0L}, i.e., to set

$$u_{0L} = v_{0L} - [Nkrj_L(kr)][-N + Nk^{-1} \int v_{0L} W\, krj_L(kr)dr].$$

This trial function satisfies (3.16) and the boundary conditions automatically, i.e., without adjustment of any parameters, but it may be unwieldy.)

It is important to recognize that the constraint imposed upon u_{0L} by (3.16) is not an unnatural one; on the contrary, as seen from (3.15), the exact function $\bar{u}_{0L}$ satisfies precisely this condition. Furthermore, for a very natural choice of the form of u_{0L} and for some very natural methods of determining the constants which characterize u_{0L}, equation (3.16) will automatically be satisfied. In particular if we write

$$(3.17) \qquad u_{0L}(r) = \cot\eta_L\, krj_L(kr) + Y_L(r),$$

where Y_L satisfies the necessary boundary conditions and depends upon various constants C_i but not on cot η_L, and if, following Kato, we choose the C_i and cot η_L by minimization of

$$(3.18) \qquad \varepsilon_{0L}{}^2 = \int \rho^{-1}(\mathcal{L}_L\, u_{0L})^2 dr,$$

minimization of $\varepsilon_{0l}{}^2$ with respect to cot η_L can readily be shown to lead to (3.16), for $\rho = W$. Similarly, for a trial function of the form given by (3.17), minimization of the entire expression for the bound on k cot η_L can also readily be shown to lead to (3.16). The latter case includes the special case for which ${}_2\beta_{0L}$ is infinite.

C. ${}_2\beta_{\theta L}$ larger than $\beta_{\theta L}$. If $0 \leq \rho = W < b/r^2$, and if $\bar{\eta}_L < \theta < \pi$, it has been shown previously[1], [2] that

$$\beta_{\theta L} \geq 1 + b^{-1}(2 - 2\theta\pi^{-1})(3 - 2\theta\pi^{-1} + 2L). \tag{3.19}$$

Under these circumstances, the evaluation of a bound on ${}_2\beta_{0L}$ consists of the determination of that value of μ for which the L-th phase shift associated with $[(1 + \mu)b - L(L + 1)]r^{-2}$ is π. This corresponds to the case $\bar{\eta}_L < \theta$ with θ approaching zero, so that from (3.19), if $0 \leq \rho = W < b/r^2$ and if $\bar{\eta}_L < \pi$,

$$ {}_2\beta_{0L} \geq 1 + b^{-1}(6 + 4L). \tag{3.20}$$

${}_2\beta_{0L}$ is at least as large as $\beta_{\theta L}$, and can be considerably larger for θ not too much smaller than π.

For a trial function of the form given by (3.17), with the parameters determined as discussed above, it is obviously preferable for $\theta = 0$ normalization to use ${}_2\beta_{0L}$ rather than β_{0L}, since one has the same trial function in each case and ${}_2\beta_{0L}$ is greater than β_{0L}.

Though it is not quite so obvious, it is still true that for such a trial function it is preferable to use ${}_2\beta_{0L}$ rather than, for example, $\beta_{\pi/2,L}$. To see this, let the upper and lower bounds on $k \cot \bar{\eta}_L$ as determined by Kato, equation (1.1), for $\theta = \pi/2$ normalization, be denoted by ub and ℓb, respectively, and let UB denote the upper bound as determined with the use of ${}_2\beta_{0L}$. Then

$$\text{UB} = k \cot \eta_L - \int u_{0L} \mathcal{L}_L u_{0L} dr + {}_2\beta^{-1}_{0L} \varepsilon^2_{0L}, \tag{3.21}$$

or

$$\text{UB} = \text{ub} - (k \cot \eta_L - \text{ub})^2(\text{ub})^{-1} - \varepsilon^2_{0L}(\beta^{-1}_{\pi/2,L} - {}_2\beta^{-1}_{0L}). \tag{3.22}$$

The use of $\theta = \pi/2$ normalization is permissible only for $\bar{\eta}_L < \pi/2$, in which case $k \cot \bar{\eta}_L$ (and therefore ub) is greater than zero, so that UB is in fact a better bound than ub. While the difference between them is only of second order, this difference may well be significant for those difficult problems for which one cannot readily obtain a good trial function.

As a concrete example, consider the evaluation of bounds on $\bar{\eta}_0$ for

(3.23) $W(r) = (2/a_o^2)[(a_o/r) + 1]\exp(-2r/a_o)$,

the 'static hydrogen potential' analyzed by Kato. He showed that $W \leq 0.5871r^{-2}$, and chose as his trial function

(3.24) $u_{00}(r) = \cos kr + \cot \eta_0 \sin kr - [1 + C_1(r/a_0)]\exp(-2r/a_0)$,

which is of the form of (3.17). If the trial function is simplified by setting $C_1 = 0$, it is found for $k = 0$ with $\theta = \pi/2$ normalization that $\gamma \equiv k \cot \eta_0 = 0.1250$ and that

$$k \cot \bar{\eta}_0 \leq 0.1096 = ub,$$

while $\theta = 0$ normalization and the use of ${}_2\beta_{00} = 11.22$ (as compared to $\beta_{\pi/2,o} = 4.407$) give

$$k \cot \bar{\eta}_0 \leq 0.1070 = UB.$$

It is known from Kato's work that for $k = 0$

$$0.10560 \leq k \cot \bar{\eta}_0 \leq 0.10598.$$

Taking the most unfavorable case, that is, assuming that $k \cot \bar{\eta}_0 = 0.01560$, we find that the difference between UB and $k \cot \bar{\eta}_0$ is only one-third of the difference between ub and $k \cot \bar{\eta}_0$ even though the calculations of UB and ub are essentially identical in that the trial functions differ only in normalization.

The values of ub for the trial function given by (3.24), with C_1 and $\cot \eta_0$ adjustable, have been tabulated by Kato for a number of values of k. Since he also tabulates $\gamma = k \cot \eta_0$, and $\varepsilon_{00}{}^2$, the values of UB can be determined immediately from (3.22). (Normally, of course, one would determine UB from (3.21).) As was noted above, the difference between UB and ub is of second order, and since we are now using a rather good trial function, the improvement in UB over ub is not so great. Even so, for the least favorable assumption as to the true value of $k \cot \bar{\eta}_0$, the improvement is about 15 °/o and is somewhat larger, as one might expect, for the value $ka_0 = 1$ for which ub - ℓb is largest, that is, in the region for which the trial function is least adequate (see Table I).

Table I

Comparison of upper bounds on k cot $\bar{\eta}_0$. ub is determined from equation (1.1), while the determination of UB depends upon the introduction of ${}_a\beta_{00}$. ℓb is a lower bound.

ka_0	ℓb	ub	UB
0	0.10560	0.10598	0.10592
0.068	0.10917	0.10952	0.10947
0.136	0.11982	0.12008	0.12004
0.272	0.16186	0.16192	0.16191
0.384	0.21629	0.21632	0.21632
0.608	0.37414	0.37468	0.37455
1.000	0.78278	0.78643	0.78564

D. Increase of the cut-off point, a. If $\bar{\eta}_0 < \theta < \pi$, and if $W(r)$ is non-negative for $r > a = k^{-1}(\pi - \theta)$, then a lower bound on $\bar{\eta}_0$ is provided by the determination of a lower bound on $\bar{\eta}_0^c$, the 0-th phase shift associated with $W^c(r)$, the latter being merely $W(r)$ but cut off at the point a, and for which the calculation is greatly simplified since $\beta_{\theta 0} = \infty$. If $W(r)$ is non-negative for all r, and if $\bar{\eta}_0 < \pi$, the introduction of ${}_2\beta_{00}$ allows one to choose $a = k^{-1}\pi$, which is considerably larger than the value $a = k^{-1}(\pi - \theta)$ for θ not too small[5].

Before proceeding to an actual application, it will be shown that, as could be expected, the increased value of a can mean a considerable reduction in the error introduced by cutting off $W(r)$ at $r = a$, i.e., a considerable reduction in $\bar{\eta}_L - \bar{\eta}_L^c$. The 'potential' given by (3.23) will again be considered, for $L = 0$. The exact expression for $\bar{\eta}_0 - \bar{\eta}_0^c$ is given by

$$(3.25) \qquad k \tan(\bar{\eta}_0 - \bar{\eta}_0^c) = \int_a^\infty W \, \bar{u}_0 \, \bar{u}_0^c \, dr,$$

where $\bar{u}_0$ and $\bar{u}_0^c$ are the exact 'absolute normalization' solutions for W and W^c, respectively. If a is sufficiently large, then $\bar{\eta}_0 \approx \bar{\eta}_0^c$, $\bar{u}_0^c \approx \bar{u}_0 \approx \sin(kr + \bar{\eta}_0)$, and r can be replaced by a in the integrand except in the exponential. (The exponential is rapidly varying and $\bar{\eta}_0$ is not too close to a multiple of $\pi/2$ for the values under consideration). Equation (3.25) becomes

$$\bar{\eta}_0 - \bar{\eta}_0^c \approx \sin^2(ka + \bar{\eta}_0)\left[(ka)^{-1} + (ka_0)^{-1}\right]\exp(-2a/a_0).$$

Since $\bar{\eta}_0 < \pi/2$ for all k for this 'potential'[1], it is permissible to set $\theta = \pi/2 = ka$ or, with the introduction of ${}_2\beta_{00}$, to set $\theta = 0$ and $ka = \pi$. Using the known values[1] of $\bar{\eta}_0$, one finds the results shown in Table II. It is clear that while either method is quite adequate for the values of ka_0 under consideration, accurate results can be obtained for somewhat larger values of ka_0 only with $\theta = 0$ normalization.

Table II

Error introduced by cutting off the potential.

A comparison of the difference between the true phase shift, $\bar{\eta}_o$, and the phase shift for the cut-off potential, $\bar{\eta}_o^c$, for L = o scattering by the potential given by equation (3.23), for the choices $\theta = \pi/2$ and $\theta = 0$, respectively. The latter choice is possible only with the introduction of ${}_a\beta_{00}$. The symbol a(-b) represents a x 10^{-b}.

ka_o	0	0.068	0.136	0.272	0.384	0.608	1.000
$\bar{\eta}_o - \bar{\eta}_o^c$, $\theta = \pi/2$	0	1(-19)	4(-10)	1(-6)	2(-4)	4(-3)	3(-2)
$\bar{\eta}_o - \bar{\eta}^c_o$, $\theta = 0$	0	4(-40)	4(-20)	3(-10)	2(-7)	4(-5)	2(-3)

The use of a cut-off potential with $\theta = 0$ normalization will then introduce a smaller error than the use of a cut-off potential with $\theta = \pi/2$ normalization, for instance. The question of whether $\theta = 0$ normalization is simple to apply will now be examined by considering L = 0 scattering by the attractive exponential potential

$$W(r) = W_0 \exp(-r/r_0).$$

(This is a solvable problem, and it will be possible to compare our results with the exact values). For $W_0 r_0^2 \leq 2$, comparison with the solvable Hulthén potential shows that $\bar{\eta}_0$ is less than $\pi/2$ for all k. We can then cut the potential off at $r = a = \pi^{-1}k$, and choose as our trial function for $r < a$

$$u_{00}(r) = \cot \eta_0 \sin kr - \sin \tfrac{1}{2}kr + \varepsilon_n C_n \sin nkr,$$

while for $r > a$ we must have an exact solution

$$u_{00}(r) = \cot \eta_0 \sin kr + \cos kr,$$

where $\cot \eta_0$ is arbitrary, but where the C_n must satisfy

$$\varepsilon_n (-1)^n n\, C_n = 0$$

in order to satisfy continuity in slope and value.

For $kr_0 = W_0 r_0^{\,2} = 1$, the true value of $\cot \overline{\eta}_0$ is 2.37; setting $C_n = 0$, variation of $\cot \eta_0$ leads to $\cot \overline{\eta}_0 \leq \cot {}^{-c}_{\;0} \leq 2.79$, while setting $C_2 = \frac{1}{2}C_1$ and $C_n = 0$ for n greater than 2 leads by variation of $\cot \eta_0$ and of C_1 to $\cot \overline{\eta}_0 \leq \cot \overline{\eta}^c_0 \leq 2.56$. As was noted earlier, the subsidiary condition imposed by equation (3.16) is automatically satisfied in these calculations. (One readily finds from (3.25) that $\overline{\eta}_0 - \overline{\eta}^c_0 \approx 0.0055$, so that it would be expected but not guaranteed that $\cot \overline{\eta}_0 = \cot(\overline{\eta}^c_0 + [\overline{\eta}_0 - \overline{\eta}^c_0])$ would be less than 2.52). Further improvements on the bound could of course be effected by the inclusion of more non-vanishing coefficients C_n.

E. $_2\beta_{\theta L}$ infinite while $\beta_{\theta L}$ finite. The cases treated thus far have specifically assumed that $W(r)$ is non-negative and that it can be shown that the phase shift of the angular momentum under consideration is less than π. The following two examples will show that these are not inherent limitations of the method. These examples will at the same time show that, as was asserted previously, there are in fact cases for which $_2\beta_{\theta L}$ is infinite while $\beta_{\theta L}$ is finite.

Thus, assume again that $W(r)$ is positive for $r \leq a$ and vanishes for $r > a$, but let it only be known that $\theta < \overline{\eta}_L < \pi + \theta$ and that $-\pi + \theta < \overline{\eta}^{\infty}_L$. For the choice $\rho = W$, $\beta_{\theta L}$ is finite and one cannot solve for $\phi_{m'L} = \phi_{oL}$ so that one cannot introduce $_2\beta_{\theta L}$, and the difficult second-order error integral would have to be evaluated. We can however choose $\rho = W - W^s$, where $W^s \geq 0$ is a square well (with range less than a) and where $W \geq W^s$. The associated differential equation introduced by Kato is readily solvable for $\mu = -1$, being simply the equation for a square well potential. For those cases for which it is possible to choose a W^s which satisfies $W^s \leq W$ and for which the phase shift associated with W^s and therefore with the then known function ϕ_{0L} is θ, the choice of a trial function which satisfies

$$b_{m'L} = b_{0L} = k^{-1} \int \phi_{\theta L} \mathcal{L}_L u_{\theta L} \, dr = 0$$

enables us to introduce ${}_2\beta_{\theta L}$, which is now infinite, thereby avoiding the difficult integration.

As an example of a case for which $W(r)$ need not be non-negative, let the only condition on $W(r)$ be that it vanish for $r > a$. Let it be known that $\theta - \pi < \bar{\eta}_L < \theta$, and that

$$\theta - 2\pi < \bar{\eta}_L^{\infty} < \theta - \pi.$$

Choose $\rho = W + W^s$, where $W^s \geq 0$ is a square well of range $\leq a$ such that $W + W^s \geq 0$. For those cases for which it is possible to choose W^s such that the L-th phase shift associated with $(-W^s)$ is $\theta - \pi$, $\phi_{-1,L}$ is known, and if $u_{\theta L}$ is chosen such that

$$b_{m'L} = b_{-1,L} = k^{-1} \int \phi_{-1,L} \mathcal{L}_L u_{\theta L} \, dr = 0,$$

we have ${}_2\beta_{\theta L} = \infty$. (If $W(r) > 0$, it will always be possible to choose such a W^s).

Formally, one can impose two subsidiary conditions on the trial function, namely, $b_{m'L} = 0$ and $b_{m'-1,L} = 0$, and introduce ${}_3\beta_{\theta L}$. While this would be very useful, the subsidiary conditions can be satisfied only if one can determine both $\phi_{m'L}$ and $\phi_{m'-1,L}$, and this does not seem to be possible.

It will occasionally be useful to introduce ${}_2\alpha_{\theta L}$, the advantage being of the kind discussed in subsection C above. Unlike the case of ${}_2\beta_{\theta L}$, however, this will never produce the major improvement of eliminating the difficult second-order error integral, for one can never have ${}_2\alpha_{\theta L} = \infty$.

4. Phase shift inequalities

It is an unfortunate feature of the Kato formalism that a certain amount of (crude) information about $\bar{\eta}_L$ is required before one can proceed to the determination of close and useful bounds on $\cot(\bar{\eta}_L - \theta)$. (The information is essential to the evaluation of $\alpha_{\theta L}$ and $\beta_{\theta L}$. Roughly speaking, $\bar{\eta}_L$ must be known to within an interval of π). This can be quite disturbing, for the Kato method is potentially most useful for precisely those very difficult problems for which one is not likely to have the requisite information, crude as that information need be. It is therefore satisfying to note that at least limited use can be made of the Kato formalism even when there is no such prior information; in particular, one will often be able to obtain a bound on $\bar{\eta}_L$ even when one cannot obtain a bound on $\cot(\bar{\eta}_L - \theta)$.

Assume, for example, that $W(r)$ is non-negative, so that $\bar{\eta}_L \geq 0$. Kato showed then that if $\bar{\eta}_L < \pi$,

$$(4.1) \qquad \cot \bar{\eta}_L \leq \cot \eta_L(S),$$

where $\cot \eta_L(S)$ is the Schwinger variational expression defined by the right side of equations (2.1) and by (2.2). However, with $\eta_L(S)$ chosen to lie between 0 and π, the requirement that $\bar{\eta}_L$ be less than π is entirely irrelevant in the determination of a bound on $\bar{\eta}_L$ from (4.1). To see this, we note that, obviously, either $\bar{\eta}_L \geq \pi$ or $\bar{\eta}_L < \pi$. In the latter case, (4.1) is valid, and it follows that $\bar{\eta}_L \geq \eta_L(S)$. In the former case, it is certainly true that $\bar{\eta}_L \geq \eta_L(S)$. It therefore follows for $W(r) > 0$, without any prior knowledge of $\bar{\eta}_L$, that

$$(4.2) \qquad \bar{\eta}_L \geq \eta_L(S).$$

On the other hand, one can not say that (4.1) is valid unless one knows that $\bar{\eta}_L < \pi$.

Equation (4.2) is in itself useless with regard to immediate application to a cross section calculation, for it places no limit on $\sin \bar{\eta}_L$. However, it can be of interest in and of itself. Further, it raises the lower bound on $\bar{\eta}_L$ from 0 to $\eta_L(S)$, so that if one has some upper bound on $\bar{\eta}_L$, one may in fact have narrowed the range of possible values of $\bar{\eta}_L$ to a width less than π; finally, if the width is still not less than π, it will be shown in Section 5 that a modified reapplication of the above technique will often enable one to raise the lower bound still more.

Equation (4.1) is a very special result of the Kato formalism, corresponding to $\theta = 0$ normalization and essentially to a particular form of trial function. More generally, it follows for $W(r) \geq 0$, if $\bar{\eta}_L < \theta < \pi$, in which case the choice $\rho = W$ leads to $\beta_{\theta L} > 1$, that

$$(4.3) \quad k \cot(\bar{\eta}_L - \theta) \leq k \cot(\eta_L - \theta) - \int u_{\theta L} \mathcal{L}_L u_{\theta L} dr + \int W^{-1} (\mathcal{L}_L u_{\theta L})^2 dr.$$

Again, it may be possible to deduce a useful bound on $\bar{\eta}_L$ *without* the knowledge that $\bar{\eta}_L < \theta < \pi$, for either $\bar{\eta}_L \geq \theta$ or $\bar{\eta}_L < \theta$. In the latter case, (4.3) is valid, and since $-\pi < \bar{\eta}_L - \theta < 0$, we are led to a result of the form $\bar{\eta}_L - \theta \geq -B$, where $0 < B < \pi$. (This is a useful result only if B is less than θ, for we knew at the outset that $\bar{\eta}_L$ was positive). If $\bar{\eta}_L$ is greater than θ, then certainly $\bar{\eta}_L \geq \theta - B$. We then have the general result for $W(r) \geq 0$, without any prior knowledge of $\bar{\eta}_L$, that

$$(4.4) \quad \bar{\eta}_L \geq 0 - B, \quad 0 < B < \pi,$$

where B is determined by setting $-k \cot B$ equal to the right side of (4.3). Again, while the consequence of (4.3), namely, (4.4), is in any event valid, equation (4.3) itself does *not* follow unless one knows that $\bar{\eta}_L < \theta$.

The above technique is clearly not restricted to the two special cases thus far considered. It is almost always possible to obtain a lower bound on the phase shift; one can, for example, compare the potential under consideration with a repulsive inverse square law potential. Provided that one can evaluate $\beta_{\theta L}$ *if* it is known that the phase shift lies within an interval θ of the lower bound, where θ is less than π, one can use this value of $\beta_{\theta L}$ in an attempt to raise the lower bound without the knowledge that the phase shift lies within the interval. If the lower bound can be raised in this manner, one can then proceed anew from the improved lower bound. In this way, one may be able, so to speak, to raise oneself by one's own bootstraps. Of course, at each step it must be possible to evaluate $\beta_{\theta L}$ under the assumption, *which need not be true*, that the phase shift lies within an interval θ of the new lower bound.

5. The bootstrap technique

To examine the bootstrap technique in more detail, and to develop it further, consider a 'potential' $W(r) \geq 0$. While ultimately it is only a bound on $\bar{\eta}_L$ that is being sought, it will prove useful to concern ourselves temporarily with bounds not only on $\bar{\eta}_L = \delta_L(0)$, but on $\delta_L(u)$ for a range of values of μ. With ρ chosen equal to W, $\delta_L(\mu)$ is the exact L-th phase shift associated with $(1+\mu)W$. For $\mu \geq -1$, it is of course true that

$$(5.1) \qquad \delta_L(\mu) \geq \delta_L(o)(\mu) \equiv 0;$$

the more significant point is that this lower bound can be raised for $\delta_L(\mu)$ with $\mu > -1$ exactly as was done above for $\delta_L(o)$. Thus, choosing $\Theta = 0$, and thinking of $(1 + \mu)W$ as the 'potential' rather than W, we write

$$(5.2) \qquad \left\{ \begin{aligned} k \cot \delta_L(\mu) \leq k \cot \delta_{tL}(\mu) &- \int u_{OL}(\mathcal{L}_L + \mu W)u_{oL}\,dr \\ &+ \int [(1 + \mu)W]^{-1}[(\mathcal{L}_L + \mu W)u_{OL}]^2 dr \end{aligned} \right\}.$$

The curly brackets around the equation signify that while the inequality itself may or may not be true, the inequality on the phase shift deduced from it is true; the curly bracket notation will be adhered to from now on. (The condition for the validity of (5.2) for any specified value of μ is of course that $\delta_L(\mu)$ be less than π, and we do not know if this is the case.) The trial function u_{OL} in (5.2) is a function of μ as well as of r, while $\delta_{tL}(\mu)$ is the trial L-th phase shift associated with $(1 + \mu)W$ and follows from the specification of u_{OL}. From (5.2), we obtain a curve $\delta_L{}^{(1)}(\mu)$ for $\mu > -1$ such that

$$(5.3) \qquad \delta_L(\mu) \geq \delta_L{}^{(1)}(\mu),$$

where $0 \leq \delta_L{}^{(1)}(\mu) \leq \pi$. Equation (5.3) is clearly an improvement upon (5.1).) In many cases, if $\bar{\eta}_L$ is greater than $\pi/2$, there will be a negative value of μ, to be called $\mu_{\pi/2,L}$, for which

$$(5.4) \qquad \delta_L{}^{(1)}(\mu_{\pi/2,L}) = \pi/2.$$

(The value $\pi/2$ is a convenient choice as will be seen shortly, but it is not a necessary choice.) Let us consider a case for which such a value of μ can be found. With $\Theta' = \pi/2$ normalization, it follows, if $\bar{\eta}_L < (3/2)\pi$, that

$$(5.5) \qquad \beta_{\pi/2,L} \geq -\mu_{\pi/2,L}.$$

This enables one to obtain an improved lower bound on $\bar{\eta}_L$, whether or not it is in fact true that $\bar{\eta}_L < (3/2)\pi$ (see Figure 2).

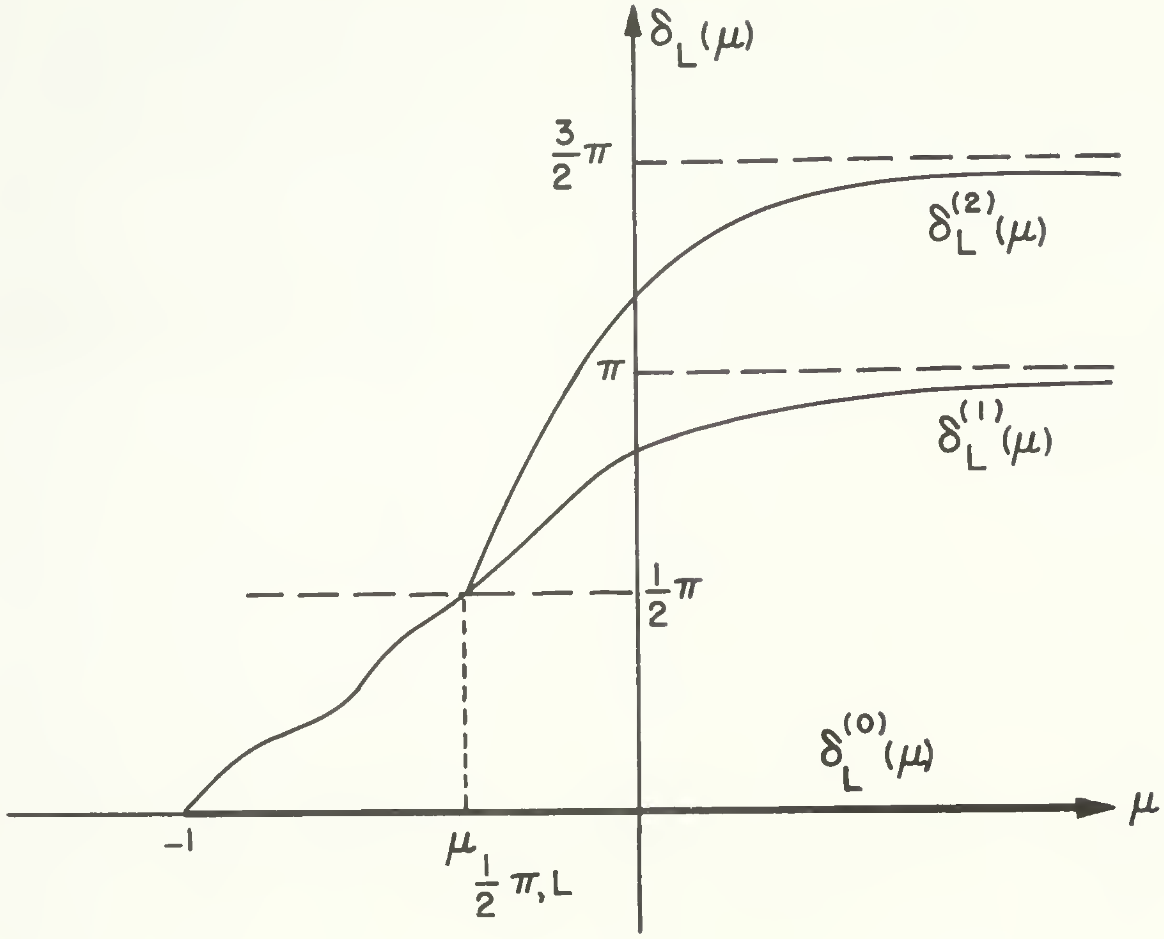

Figure II

A schematic representation of the 'bootstrap technique' for raising the lower bound on $\bar{\eta}_L$. The sequence of curves $\delta_L^{(0)}(\mu)$, $\delta_L^{(1)}(\mu)$, etc., represent successively better lower bounds on $\delta_L(\mu)$. The bound on $\bar{\eta}_L$ is determined from the relationship $\bar{\eta}_L = \delta_L(0)$.

As a concrete example, consider $L = 0$ scattering by

$$W(r) = W_o \exp(-r/r_o). \tag{5.6}$$

With $\theta = 0$, and with the choice

$$u_{oo}(\mu,r) = \cos kr + \cot \delta_{to}(\mu) \sin kr - y(\mu,r), \tag{5.7}$$

where $y(\mu,o) = 0$ and where $y(\mu,r) \rightarrow 0$ as $r \rightarrow \infty$, equation (5.2) reduces to

$$\left\{ k \cot \delta_o(\mu) \leq - \int (y'^2 - k^2 y^2) dr + \int \left[(1+\mu)W\right]^{-1} (y'' + k^2 y)^2 dr \right\}.$$

Choosing

$$y(\mu,r) = \left[1 + C(r/r_o) + D(r/r_o)^2\right] \exp(-r/r_o),$$

where C and D can be functions of μ, we find, for $kr_o \rightarrow 0$,

$$\left\{ kr_o \cot \delta_o(\mu) \leq f(C,D) \left\langle 1 - g(C,D) \left[(1+\mu) W_o r_o^2\right]^{-1} \right\rangle \right\}, \tag{5.8}$$

where

$$f(C,D) = - \frac{1}{4}(2 - 2C + C^2 - 2D + D^2 + CD), \tag{5.9}$$

and where

$$g(C,D) = -(1 - 2C + 2C^2 + 4D^2)/f(C,D). \tag{5.10}$$

It follows from (5.3) and (5.4) that $\mu_{\pi/2,0}$ is that value of μ for which the right side of (5.8) vanishes. (It is the fact that the right side then vanishes, which is the convenience, mentioned earlier, associated with the choice $\theta = \pi/2$.) From (5.5) and (5.8), we then find

$$\beta_{\pi/2,o} \geq -\mu_{\pi/2,0} = 1 - 1.456(W_o r_o^2)^{-1},$$

where 1.456 was obtained by maximizing $g(C,D)$, defined by equations (5.9) and

(5.10). Equation (5.9) has meaning only if $\beta_{\pi/2,o}$ is greater than 0, that is, only if $W_o r_o^2 > 1.456$.

We now fix our attention upon the particular numerical value $W_o r_o^2 = 25/4$. The exact solution for $kr_o \rightarrow 0$ is then* $\bar{\eta}_o \rightarrow \pi + 2.470\ kr_o$, so that $\tan \bar{\eta}_o /(kr_o) \rightarrow 2.470$. Equation (5.9) gives $\beta_{\pi/2,o} \geq 0.76704$. (The exact value of $\beta_{\pi/2,o}$, which in this case is that value of β for which the phase shift associated with $(1 - \beta)W_o$ is $\pi/2$, is 0.7686.) Note, incidentally, that we now know that $\bar{\eta}_o = \delta_o(o) > \delta_o(\mu_{\pi/2,o}) \geq \pi/2$. We take a trial function of the form used for example by Huang[5], but with $kr_o \rightarrow 0$, and normalized to $\theta = \pi/2$, that is,

$$(5.11) \qquad (-kr_o)^{-1} u_{\pi/2,o} = X + C_1 - (C_1 + C_2 X + C_3 X^2 + C_4) \exp(-X) + C_4 \exp(-2X),$$

where $X = r/r_o$, and where C_1 is to be thought of as $(1/kr_o)$ times the tangent of the trial phase shift. This trial function was used in equation (1.1), first neglecting and then including the $(1/\beta)$ term, that is, in an ordinary variational calculation, and in a calculation which gives a 'curly bracket lower bound' on $\tan \bar{\eta}_o/(kr_o)$. The bound is of a curly bracket type because we proved that $\bar{\eta}_o$ was greater than $\pi/2$, but simply assumed that $\bar{\eta}_o$ was less than $(3/2)\pi$. The bound deduced on $\bar{\eta}_o$ is of course nevertheless guaranteed to be correct.

The coefficients in the calculation of the bound were determined by minimizing the entire expression for the bound rather than by minimizing ε^2. There is no point to the latter procedure here, for it is no simpler than the former and must give a poorer bound on $\tan \bar{\eta}_o/(kr_o)$. Further, that procedure negates one of the very pleasant features associated with the appropriate use of the Kato formalism;

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*cf. Morse and Feshbach[4], p. 1688. Note, however, that these authors are not concerned with multiples of π, while we are, in the present work.

in particular, if one minimizes the entire expression for the bound, the inclusion of more parameters in the trial function can only improve the bound, while if one minimizes ε^2, the inclusion of more parameters may make the bound worse. (The situation in the latter case is then of the same nature as that of the usual variational calculation). Of course, one might still minimize ε^2 if one were primarily interested in an accurate wave function rather than in an accurate bound.

The results, shown in Table III, are about as might be expected. Since the true value of $\bar{\eta}_0$ is greater than π, a number of coefficients are required even for the variational calculation to give accurate results; the bound, arising from a vigorous expression, is rather conservative. (On the other hand, for somewhat smaller values of $W_0 r_0^2$, quite accurate results are obtained for the bound as well as for the variational result with three or even two parameters in the trial function).

The only rigorous statement that follows from the calculations is that $\bar{\eta}_0$ is greater than $\pi + 2.0' kr_c$. In practice, however, the four parameter calculations show, through the fair degree of consistency of the four values of C_1, C_1, the variational value of $\tan \bar{\eta}_0/(kr_0)$ and the bound on $\tan \bar{\eta}_0/(kr_0)$, and through the smallness of ε^2, that in fact one could be fairly certain that the true value of $\tan \bar{\eta}_0/(kr_0)$ or $(\bar{\eta}_0 - \pi)/(kr_0)$ is close to 2.45, the variational estimate. This would be the case even if we could not obtain some upper bound on $\bar{\eta}_0$.

From the point of view of this section, however, the most interesting result of these calculations is that it has been possible to raise the lower bound significantly, in particular above π, without recourse to a knowledge of the phase shifts associated with any other potential. In effect, we have used as our comparison potential the potential under consideration, but with varying strength.

In principle, one can introduce $\delta_L^{(2)}(\mu)$ and higher curves, but in practice this would probably not be a reasonable procedure.

The discussion of Sections 4 and 5 can also be immediately applied to the case in which one has an upper bound on $\bar{\eta}_L$ and $\sigma_{\theta L}$ is determinable under the assumption that $\bar{\eta}_L$ lies within an interval θ of this upper bound, where θ is less than π.

TABLE III. Variational calculation of $\tan \bar{\eta}_0$ and calculation of bound on $\bar{\eta}_o$.

(1) case	(2) C_1	(3) C_2	(4) C_3	(5) C_4	(6) variational calculation of $\tan \bar{\eta}_o/(kr_o)$	(7) Lower bound on $(\bar{\eta}_o-\pi)/(kr_o)$	(8) $\frac{\varepsilon^2(\pi/2),0}{k^2 r_o^2}$
(a)	-	-	-	-	+12.500	-3.7964	+12.500
(b)	-2.9603	-	-	-	-1.377	-	-
(c)	+0.72659	+9.4581	-	-	+1.147	-	-
(d)	+2.3834	+10.041	+2.6548	-	+1.761	-	-
(e)	+2.2944	+35.178	-4.8426	-26.281	+2.45	-	-
(f)	-3.1886	-	-	-	-	-3.4140	+1.6252
(g)	+16.122	+10.324	-	-	-	-0.835	+276.68
(h)	+10.772	+8.2011	+0.76605	-	-	-0.651	+125.96
(i)	+1.0480	+28.541	-2.9300	-20.715	-	+2.08	+1.26

Scattering by $W(r) = W_o \exp(-r/r_o)$ for $L = 0$, $kr_o \rightarrow 0$, $W_o r_o^2 = 25/4$. The trial function is given in equation (5.11). The calculation does not use any solvable comparison potentials. The coefficients C_1 through C_4 for cases (b) through (e) were calculated from the Kato variational principle with $\theta = \pi/2$; this is precisely the Kohn variational principle. The coefficients for cases (f) through (i) were chosen by minimizing the bound. The true values are $\tan \bar{\eta}_o/(kr_o) \rightarrow 2.470$ and $(\bar{\eta}_o - \pi)/(kr_o) \rightarrow 2.470$.

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25 Waverly Place
New York 3, N. Y.